crucially important for antitumor immunity. In cancer, DCs accumulate lipids and form lipid droplets (LD) - dynamic organelles composed of hydrophobic core of neutral lipids covered by monolayer of phospholipids. This is associated with the suppression of CP function of DCs. We detected and identified several molecular species of oxidized neutral lipids, particularly tri-acylglycerols (oxTAGs), cholesterol esters (oxCH) and free fatty acids (oxFFAs) lipids) accumulating in LDs of DCs in tumor bearing hosts. We further established that these oxidized neutral lipids are causatively linked to the suppression of CP. To get further insights into mechanisms of this effect we performed computational modeling using two different methods. The coarse-grained molecular dynamics simulations (CGMD) demonstrated that oxTAGs with polar oxygenated groups in their acyl chains redistributed from the hydrophobic core to the polar surface areas of LDs. Molecular docking analysis of interactions of ovalbumin (OVA) as an antigen with neutral lipids revealed separate high affinity binding sites for TAG and oxTAG. The binding energy for oxTAG was ~35% higher than for non-oxidized TAGs suggesting a strong binding of the antigen with oxidized lipids on the surface of LDs. These results are compatible with our hypothesis that oxidized neutral lipids of LDs are involved in the suppression of antigen CP in cancer. This work was supported by NIH grants R01CA165065.

4065-Pos Board B793

A Software Platform for Finite Element Simulation of Ion Permeation in Ion Channel Systems

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As it is hard to apply all-atomic model to simulate the whole process of ion permeation in ion channel, we use continuum electrodiffusion description for ion flow in the channel system. Electrodiffusion process exists in many apparently different physical objects such as electrolyte cell, nanofluidic device, charged porous media, and ion channel in biology. Real 3D ion channel is particularly difficult to simulate due to the multiscale nature of the transport process, the complex geometry/boundary of the channel protein system, and the singular charge distribution inside the channel protein(s). For this reason, there are so far only a very few softwares publicly available in this important area of biology. We will show our recent relevant works and plan to build up such a platform. In the first part, we'll talk about the continuum models and numerical works. They include the Poisson-Boltzmann equation, the Poisson-Nernst-Planck equations and their improved forms, and some efficient algorithms we developed for the solution of these equations. In the second part, we will describe the molecular meshing problem which is essential for finite/boundary element modelings. We recently developed a novel and robust mesh generation tool TMSmesh that can handle complex and arbitrarily large biomolecular system. In the third part, I will give a brief introduction to an undergoing project of designing a visualization system, VCMM, to facilitate researches in this area. Finally, we will show applications using our parallel finite element solver to compute properties such as current-voltage characteristics (curves) and conductance to a few channel systems. The results agree well with those obtained with Brownian Dynamics simulations and experiments.

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Heterogeneity of Threadlike Shape of DNA-Stabilized Silver Fluorescent Clusters

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DNA is widely used as a stabilizing matrix in the synthesis of fluorescent silver nanoclusters (AgNCs) possessing good biocompatibility and high brightness. We studied a group of threadlike shaped clusters up to 8 atoms having an elongated shape, so that each atom is connected with only one or two neighbors. Such the choice have been proved by recent calculations of electronic excitation spectra of threadlike shaped silver clusters showing intense the lowest transition, energy of which depends strongly on the chain bend [1]. These properties are in a good agreement with a special feature of the experimental luminescence excitation spectra of Ag clusters stabilized by polymer matrix. The formation of elongated forms of clusters necessarily involves several binding sites regularly arranged on DNA. Following this approach we calculate geometry and electronic excitation spectra of threadlike silver clusters bound to the minor groove of polyC oligomer containing an ordered arrangement of the carbonyl oxygens as binding sites using density functional theory method. We also performed MD calculations for polyC oligomer in water-ionic solution. Conformational dynamics of DNA backbone causes the different equilibrium states of the clusters chain bend, which provides a large variety of emitting species.

1. Ruslan R. Ramazanov, Alexei I. Kononov. Excitation Spectra Argue for Threadlike Shape of DNA-Stabilized Silver Fluorescent Clusters. J. Phys. Chem. C, 2013, 117 (36), pp 18681-18687.

4067-Pos Board B795

In Silico Single-Molecule Manipulation of Chromatin Fibres with Game Engines

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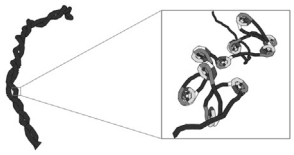
We develop a new powerful method to reproduce in silico single-molecule manipulation. We demonstrate that flexible polymers like DNA or chromatin fibres can be simulated using game engines thanks to an original implementation of Langevin dynamics in the open source library called Open Dynamics Engine. We moreover implement a global thermostat which accelerates the simulation sampling by two orders of magnitude. We retrieve force-extension as well as rotation-extension diagrams of reference experimental studies. Finally, we extend the model to simulations of chromatin loops tethered to the nuclear membrane.



4068-Pos Board B796

Interpolation of Potential Energy Surfaces for Nonadiabatic Simulations of Biological Systems

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Simulations of photophysical processes in biological systems are essential for understanding the role of molecular environment regarding the utilization of the light energy. However, such simulations are challenging in part due to the associated high computational costs, especially with the often adopted *ab initio* calculations of excited state potential energy information. Here, an application of a scheme for interpolating diabatic Hamiltonian matrix will be presented. We will show that this method is applicable for a sizeable molecular system (with 21 atoms) with a capability of describing the conical intersection properly and with an extensibility to condensed phase situations, by testing it with a model analytic potential energy surface of the green fluorescent protein chromophore. A procedure for using high-level quantum chemical calculations in the interpolation of diabatic Hamiltonian will also be presented together with the results of trajectory hopping simulations. Finally, we will discuss how this approach can be applied to computational studies of other photobiological systems.

4069-Pos Board B797

Mixed Quantum-Classical Study of the Nonadiabatic Dynamics in Photosynthetic Systems

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Quantum mechanics often participates importantly in the dynamics of biological systems. Understanding such an aspect becomes crucial when investigating nonadiabatic events within biological molecular complexes. Indeed, nonadiabaticity is an essential element in many fundamental processes such as electron and energy transfers. However, due to the immense size of any biological system, purely quantum mechanical descriptions are simply intractable. For this reason, mixed quantum-classical approaches, where an important part of the system is handled quantum mechanically and its remainder is treated through relatively simple classical mechanics, have become widely applied. Poisson bracket mapping equation (PBME), as an example of the mixed quantum-classical approach, is an attractive scheme with its applicability even to very large systems. Here, we show that PBME can be efficiently applied to studying photosynthetic energy transfer processes and to elucidating the detailed role of the surrounding protein. We will also discuss its limitations in comparison with the results of a more rigorous approach. We will also propose a simple scheme to improve the long-time behavior of PBME in terms of correct population distributions. Future prospects will also be discussed.